

# Simulation Support for Fast and Accurate Large-Scale GPGPU & Accelerator Workloads

Vishnu Ramadas, Matthew Poremba, Bradford M. Beckmann, Matthew D. Sinclair  
University of Wisconsin-Madison, AMD Research  
vramadas@wisc.edu Matthew.Poremba@amd.com Brad.Beckmann@amd.com sinclair@cs.wisc.edu

## I. INTRODUCTION

In recent years deep neural networks (DNNs) have emerged as an important application domain driving the requirements for future systems. As DNNs get more sophisticated, their compute requirements and the datasets they are trained on continue to grow at a fast rate. For example, Gholami showed that compute in Transformer networks [1] grew 750X over 2 years [2], while other work projects DNN compute and memory requirements to grow by 1.5X per year [3], [4]. Given their growing requirements and importance, heterogeneous systems often add machine learning (ML) specific features (e.g., TensorCores) to improve their efficiency. However, given ML’s voracious rate of growth and size, there is a growing challenge in performing early-system exploration based on sound simulation methodology.

Traditionally, architectural simulators are used to perform early exploration for this type of research. However, detailed simulation of modern systems can take extremely long times in existing tools. Furthermore, prototyping optimizations at scale can also be challenging, especially for newly proposed accelerators. Although tools such as Accel-Sim [5], [6], Gemini [7], MGPUSim [8], [9], and SCALE-Sim [10] enable some early experiments, they are limited in their ability to target a wide variety of accelerators and often focus on specific accelerators instead of system-wide behavior. Likewise, approaches like Path Forward [11] and Photon [12] reduce GPU simulation time by approximating the ML application behavior. However, these approaches focus on existing hardware – prototyping new optimizations on them would be challenging.

In comparison, gem5 [13], [14] has support for various CPUs, GPUs, and other important accelerators [15]–[18]. However, efficiently simulating large-scale workloads on gem5’s cycle-level models requires prohibitively long times. Accordingly, we are enhancing gem5’s support to make these workloads practical to run while retaining accuracy. This will enable users to use the same early exploration platform, gem5, for both homogeneous and heterogeneous systems. Specifically, we are extending gem5’s existing simulation infrastructure to create a scalable simulation framework that models diverse system components with varying levels of detail. We will also develop novel mechanisms that identify the most important parts of the applications to simulate at high fidelity while reducing simulation time and add support for multi-chiplet and multi-node (e.g., multi-GPU and multi-accelerator) simulations to drive a flexible, adaptable simula-

tion infrastructure that enables rapid prototyping of different optimized AI and ML algorithms and architectures while ensuring that the changes are representative of real, modern hardware and software.

## II. BACKGROUND

The gem5 simulator is a widely used, open-source, cycle-level computer system simulator. At its core, gem5 contains an event-driven simulation engine. On top of this simulation engine gem5 implements a large number of models for system components for CPUs (out-of-order designs, in-order designs, and others), GPUs (AMD and ARM models), accelerators [17], [19], various memories, on-chip interconnects, coherent caches, I/O devices, and many others. Moreover, gem5 provides two modes: Syscall Emulation (SE) and Full System (FS). SE mode simulates an application’s user mode code in detail but emulates the OS instead of simulating it in detail. Conversely, FS mode simulates both the OS and user mode code in detail, allowing users to study the interaction between the OS and architecture.

Our recent work enhanced and updated gem5’s GPU support [20] to add support for multi-chiplet setups [18] and ML workloads [16], [21] in gem5’s SE mode. However, this support focuses on relatively smaller ML workloads such as DNNMark [22] and DeepBench [23] which call ML libraries directly (unlike high-level frameworks like PyTorch or TensorFlow). To improve on this, we recently released support for running ML models in gem5’s FS mode in gem5 v23.1. As a result, users can now run PyTorch and TensorFlow workloads on CPU-GPU systems in gem5 using modern versions (e.g., v6) of AMD’s open-source ROCm stack. Unfortunately, running ML models from these high-level frameworks in gem5 is extremely slow: it would take roughly 78 days of simulation time to reach the region of interest in massive modern ML workloads running in PyTorch or TensorFlow. Thus, significant work is needed to practically simulate these large ML workloads in gem5.

## III. ON-GOING WORK

Here we discuss our on-going efforts to improve gem5’s support to practically run ML workloads and other large-scale workloads (e.g., from high performance computing). These optimizations, which we have open sourced to the public, mainline gem5 codebase, trade-off fidelity for less important portions of the workload for improved simulation time, without compromising correctness. Moreover, we are

currently working on ways to further extend this to improve simulation speed without compromising accuracy.

**Reduce Fidelity for Less Important Workload Portions with KVM:** We extended gem5’s KVM CPU support to speed up simulation for gem5 applications running on CPUs, GPUs, and other accelerators. We currently harness gem5’s KVM CPU to simulate the CPU code of a GPGPU workload at native speed on the underlying machine. We simulate the workload kernels at high fidelity using gem5’s GPU models while using the KVM CPU for everything else. However, even after doing so, if an application has several iterations or a large number of phases (e.g., GPU kernels or application phases) that require high fidelity simulation, further optimizations are required [5], [11], [12].

**Checkpoint Save/Restore Support:** We also added support for checkpointing applications and are adding support to allow gem5 users to create their own checkpoints and restore from them. For example, users could create a checkpoint for the state of the system immediately before a region of interest (ROI) executes or immediately before the first non-setup phase executes. The checkpointed state can then be restored during later simulations to skip over all instructions until the annotation and effectively begin simulating from the ROI onwards. This significantly improves simulation time by only simulating these less important parts (e.g., if a user does not care about reading inputs in [24]–[26]) once. Furthermore, for GPU phases the ROCm stack can also be modified to generate a checkpoint from hardware that contains all the required state information, and recent work has demonstrated that similar support exists for CPUs [27]. This checkpoint can then be used with gem5 to start a simulation directly from the ROI.

**Fast Forward Through Less Important Phases:** We propose to identify and fast forward through less important application phases (e.g., start-up GPU kernels). Here, like prior work, we observe that some code regions in a workload are more important to the application’s overall behavior than others. By converting less important GPU kernels to CPU phases that can be executed natively via KVM or by executing them by passing through the host machine’s GPU itself, we can simulate the workload much faster by focusing the high fidelity simulation on the most important application phases. Our initial prototype (using HIP-CPU [28] and simple GPGPU benchmarks from Rodinia [29], [30]) shows this approach is highly effective – gem5’s simulation time is only  $1.6\times$ – $3\times$  slower than bare metal (versus at least  $200\times$  slower without these optimizations). Moving forward, we plan to leverage the fact that high level frameworks have multiple backends for kernels. Accordingly, applying this to large-scale ML workloads will make their simulation tractable – allowing relatively small ML workloads to complete very quickly and making it possible to simulate much larger workloads that currently have infeasibly long runtimes. However, significant challenges exist for generating and migrating the state needed to initiate cycle-level simulation after the fast forward phase.

**Annotating Applications:** Fast forwarding through less important phases requires a simple mechanism to identify which

phases/GPU kernels are most important. To do this, we will initially manually annotate applications to identify which kernels require high fidelity. However, this may not be feasible for larger workloads. Therefore, we will develop a novel profiling scheme that analyzes large-scale ML workloads on real machines and identifies which ROIs are most important to simulate in high fidelity – by passing this information into a scripting framework we will develop, we can automatically identify the most important regions without requiring manual annotation. By utilizing the aforementioned annotations for the ROIs, we can also make it easy for users to create checkpoints for ML workloads. Here, we propose to start with our prior work on SeqPoints [31], which identifies a subset of the computation in RNNs and Transformers that are representative of the larger ML training computation. Applying SeqPoints to gem5 will create a set of profiles and checkpoints representative of the larger workloads that can be run in gem5. Our analysis shows that these profiles are up to  $345\times$  smaller than the entire ML workloads, enabling significant savings for RNNs and Transformers. For other important ML workloads, we will either adopt state-of-the-art approaches (e.g., only simulating a single CNN iteration [32] or using clustering [5]) or perform a detailed analysis of the workloads to identify what subset of the workload must be simulated at high accuracy.

**Turnkey Ease of Use:** One of the barriers to entry with using simulators such as gem5 is the difficulty in getting the tools set up properly initially. Although recent work has helped improve this [16], [21], it does not work with our proposed work. We have begun developing detailed documentation for guiding users to setup their simulation environments. We also plan to include a new chapter in the learning gem5 book as well as example applications and uses in gem5-resources [21]. These resources will allow new users to simply start running PyTorch or TensorFlow applications without worrying about how to properly configure gem5, and give them the tools needed to create their checkpoints for additional applications.

#### IV. METHODOLOGY

We will evaluate our proposed work in the gem5 simulator, and plan to continue open-sourcing this work. Our main metrics for evaluation will be a) simulation time (wall clock time) compared to the current gem5 support for these applications and b) accuracy (i.e., how well the simulated support models the behavior of applications on a given system). Here, we will leverage our recent work on improving the accuracy of gem5’s models [33], [34]. Directly quantitatively evaluating its efficacy compared to prior work (discussed in Section I) is challenging since each uses a different simulator or ecosystem. Moreover, our work evaluates the entire application, end-to-end, whereas prior work specifically analyzes the accelerator portion (e.g., the GPU kernels). However, where possible we plan to both use the same/similar applications as PKA [5], Photon [12], and Path Forward [11] to demonstrate how our findings agree and contrast.

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